Quantal statistical phase factor accompanying inter-change of two identical particles

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It is shown that the effects of particle statistics entail reduction in the number of orbital degrees-of-freedom in non-relativistic 2-particle systems from 6 to 5. The effect of redundancy in the description of orbital motion is found to be in correspondence to the multiplicative phase factor $(-1)^{2s}$ which accompany two-particle interchange, where s is the spin of one particle.

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I. INTRODUCTION

The Pauli exclusion principle is basic principle in physics, in particular it is usually related to the explanation of the shell structure of atoms, conductivity of metals, stability of matter, description of the properties of white dwarfs, and other phenomena that are of experimental and theoretical interest.

A paper by Berry and Robbins has shown that the Pauli exclusion principle may originate due to non-trivial kinematics of the electronic spins [1]. Later, it was found that this construction is not unique [2], and alternative constructions of the exclusion principle are possible. However, an earlier paper by Berry and Robbins [3] has considered a model $M = 0$ spin system in external magnetic field, and derived the phase factor $(-1)^S$ multiplying the wave-function of the model system, when the direction of the magnetic field $\mathbf{B}$ is reversed. It was shown that the configuration space of the spin system is equivalent to the configuration space of two identical particles as constructed in Ref.[4]. The derivation in Ref. [3] shows that connection between spin and statistics can be derived, rather than postulated. In different papers [5, 6], a unique connection between spin and statistics for spin $S = 0$ bosons was derived, based on the identification of the symmetric points $(\mathbf{r}_1, \mathbf{r}_2)$ and $(\mathbf{r}_2, \mathbf{r}_1)$ in the configuration space of the two particles and exploiting the continuity of the boson wave-function. In a related paper [7], the connection between spin and statistics is shown to follow if the description of the dynamics involves explicitly anti-commuting Grassmann variables. On the other hand it is known that gauge structure appears in simple classical and quantum mechanical systems [8]. It has been shown that long range forces in di-atom systems are mediated by monopole-like gauge fields [9]. Further elaboration by Jackiw [10, 11] has shown that symmetries of dynamic systems can be affected in presence of monopole gauge fields. It is therefore reasonable to look for a connection between spin and statistics in simple systems with two constituent particles.

In Ref. [12], three-dimensional variational equation of motion for N Coulombically interacting electrons was derived, which is different from the conventional $3N$-dimensional many-body Schrödinger equation. Unless otherwise stated, we use atomic units ($e = m_e = \hbar = 1$).

The non-relativistic variational Schrödinger equation of motion for one active electron in presence of identical spectator particle, and in absence of external (nuclear) forces is given by [12]

$$\left(-\frac{1}{2}\nabla^2_{\mathbf{r}_1} + \frac{g}{r_{12}} - \lambda\right)\psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = 0, \qquad (1)$$

where $g = 1/2$, $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ is the relative distance between the spectator electron placed at $\mathbf{r}_2$ and the active electron located near $\mathbf{r}_1$, σ_1 and σ_2 are the components of the electronic spins $s = 1/2$ on an arbitrary but fixed spatial $z-$axis and λ is unknown Lagrange multiplier. The variational two-body fermion amplitude is given by

$$\psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = \langle \mathrm{vac}|\Psi(\mathbf{r}_1\sigma_1)\Psi(\mathbf{r}_2\sigma_2)|\Psi\rangle, \qquad (2)$$

where $\Psi(\mathbf{r}\sigma)$ is an anti-commuting fermion field operator, $|\mathrm{vac}\rangle$ is the vacuum state of non-interacting fermions and $|\Psi\rangle$ is unknown state-vector of the interacting system of two electrons. Since the fermion field operators anti-commute, then wave-functions of electronic states in Eq.(2) are anti-symmetric, i.e.

$$\psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = -\psi(\mathbf{r}_2\sigma_2, \mathbf{r}_1\sigma_1), \qquad (3)$$

The subsidiary condition of Eq.(3) provides the description of the dynamics of the spectator electron, which otherwise is undetermined. That is because, if $\psi(\mathbf{r}\sigma, \mathbf{r}'\sigma')$ is a solution of Eq.(1), then the re-definitions

$$\psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) \to \sum_{\lambda_1\lambda_2} U^{\sigma_1\sigma_2}_{\lambda_1\lambda_2}(\mathbf{r}_2)\psi(\mathbf{r}_1\lambda_1, \mathbf{r}_2\lambda_2), \qquad (4)$$

are also solutions of Eq.(1), where $U^{\sigma_1\sigma_2}_{\lambda_1\lambda_2}(\mathbf{r}_2)$ is an arbitrary 16-element spinor matrix, which can depend locally on the position-vector of the spectator electron, i.e. the phase and the amplitude of the wave-function are not fixed by the equation of motion alone. The physical solutions of Eq.(1) are fixed by the Pauli's exclusion principle of Eq.(3), which fixes the amplitude, the phase and the inter-relation between the components of the electronic spins of the two-electron wave-function, which otherwise remain arbitrary and undetermined. However, since the

state-vector $|\Psi\rangle$ is defined up to a global phase, the relation of Eq.(3) can be written in more general way as

$$\psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = e^{i\theta}\psi(\mathbf{r}_2\sigma_2, \mathbf{r}_1\sigma_1), \tag{5}$$

i.e. the two wave-functions are identical up to a global phase-factor, independently on the fact that the fermion field operators anti-commute. In the particular case, when $\theta = \pi$, Eq.(3) is reproduced, i.e. the particle statistics phase does not have a direct physical meaning, unless the system undergoes a cycle in configuration space, such that θ represents the phase difference between initial and final state wave-functions.

In the more general case of N-Coulombically interacting electrons in presence of external one-body potential $U(\mathbf{r})$ [12], Eq.(1) together with the subsidiary condition of Eq.(3), generalizes to one-electron equation of motion

$$\left(-\frac{1}{2}\nabla^2_{\mathbf{r}} + U(\mathbf{r}) + g\sum_{k=1}^{N-1}\frac{1}{|\mathbf{r}-\mathbf{r}_k|} - \lambda\right)\psi(\mathbf{r}\sigma, \{\mathbf{r}_k\sigma_k\}) = 0, \tag{6}$$

together with $N!-1$ symmetry constraints

$$\psi(1, 2, \dots N) = \eta_P\psi[P(1), P(2), \dots P(N)] \tag{7}$$

for anti-symmetry of the fermion wave-function due to the Fermi-Dirac statistics, by $(i) = (\mathbf{r}_i\sigma_i)$ we have denoted the coordinates of the i-th electron. The quantal statistical phase-factors $\eta_P = (-1)^P$ accompanying the inter-change of fermions are $+1$ if the permutation of the coordinates involves even number of transpositions and -1 otherwise, and $N!$ is the number of elements in the symmetric group S_N. The subsidiary conditions for anti-symmetry define the structure of the Hilbert space of N-electron wave-functions. The Hamilton equation of motion, together with the subsidiary conditions that the wave-function has to satisfy, correspond to Dirac's formulation of the constrained quantum dynamics [13]. The constraint Hamiltonian approach, has not found realization and application in solving non-relativistic problems, such as the calculation of the energy levels of the light hydrogen, helium and lithium-like atoms and ions. The purpose of this paper is compute the properties of the hydrogen and helium iso-electronic sequences, and compare these results to the experiment.

A. Theoretical formulation

The state of the interacting N-electron system can be obtained by solving a set of one-particle constraint equations for equal sharing of the total energy by the particles

$$\chi_a|\psi\rangle = 0, \quad a = 1, \dots N \tag{8}$$

where

$$\chi_a = \frac{1}{2}\mathbf{p}_a^2 + v_s(\mathbf{r}_a) - \lambda \tag{9}$$

are the operators of the constraints, λ is uniform Lagrange multiplier, $v_s(\mathbf{r})$ is the potential energy of the active electron in an external field $U(\mathbf{r})$ and including the repulsive Coulombic field of the spectator electrons

$$v_s(\mathbf{r}_a) = U(\mathbf{r}_a) + \frac{1}{2}\sum_{b\neq a} r_{ab}^{-1}, \tag{10}$$

and $r_{ab} = |\mathbf{r}_a - \mathbf{r}_b|$ denote the relative distances between particles. In addition there are N first-class constraints for identity of the particle spins, which are

$$\mathbf{s}_a^2|\psi\rangle = s(s+1)|\psi\rangle, \quad a = 1, \dots N \tag{11}$$

where $s = 1/2$ is the spin of one electron, but otherwise s can be regarded arbitrary. The particle spin operators satisfy canonical commutation relations

$$[(\mathbf{s}_a)_i, (\mathbf{s}_b)_j] = i\delta_{ab}\varepsilon_{ijk}(\mathbf{s}_a)_k. \tag{12}$$

The constraints in Eq.(8) are all second-class, since

$$[\chi_a, \chi_b] = \frac{\mathbf{r}_{ab}}{r_{ab}^3}\cdot\mathbf{P}_{ab} \neq 0, \tag{13}$$

where $\mathbf{P}_{ab} = \mathbf{p}_a + \mathbf{p}_b$ is the momentum of the center-of-mass motion of the electrons in the (a, b)-th pair. The constraints are asymptotically first-class, since they decay with inter-particle distances as r_{ab}^{-2}. The second-class constraint system can be viewed as a result of gauge-fixing in an extended first-class constraint system with gauge invariance. We consider $N = 2$, but we also consider $N = 1$, since in this particular case the present approach reduces exactly to the one-particle Schrödinger equation.

B. Motion of one free electron

By neglecting temporary the spin constraint, the Schrödinger equation of motion in momentum representation is given by

$$(\mathbf{p}^2 - 2E)\psi_E(\mathbf{p}) = 0, \tag{14}$$

where the momentum $\mathbf{p}$ of the particle is a multiplication operator. The Schrödinger equation is invariant under local change of the phase of the wave-function

$$\psi(\mathbf{p}) \to \psi(\mathbf{p})e^{if(\mathbf{p})}, \tag{15}$$

since the momentum $\mathbf{p}$ does not change

$$e^{if(\mathbf{p})}\mathbf{p}e^{-if(\mathbf{p})} = \mathbf{p} \tag{16}$$

The phase of the free-particle wave-function is therefore uncertain at each point in momentum space. Apart from the local phase invariance, there is additional type of invariance of the Schrödinger equation under s-wave redefinition of the wave-function, i.e.

$$\psi(\mathbf{p}) \to \psi(\mathbf{p}) + c(E)\delta(p - \sqrt{2E}) \tag{17}$$

does not change the equation of motion. Therefore free-particle states are defined up to an s-wave, which is a consequence of the identity $(p^2 - k^2)\delta(p-k) \equiv 0$. Therefore apart from conventional symmetries of the one-particle Hamiltonian, Schrödinger equation exhibits two additional gauge symmetries, it is invariant under local $U(1)$ phase transformations and under s-wave redefinitions of the wave-function. The Hilbert space of states is a quotient space,

$$\mathcal{H}_{\rm phys} = \mathcal{H}/\mathcal{H}_{\rm s-wave}. \qquad (18)$$

The states that are invariant under s-wave transformation of the wave-function are

$$|\psi_{\rm phys}\rangle = |\psi\rangle - \langle E, l=0, m=0|\psi\rangle |E, l=0, m=0\rangle, \qquad (19)$$

for some $|\psi\rangle \in \mathcal{H}$, i.e. $\langle \psi_{\rm phys}|E, l=0, m=0\rangle = 0$, and hence the free-particle states do not contain s-wave component. Two states are gauge-equivalent, if they differ only by an s-wave

$$|\psi\rangle \sim |\psi\rangle + c(E)|E, l=0, m=0\rangle. \qquad (20)$$

To obtain free-particle wave-functions, gauge fixing-conditions $C|\psi\rangle = 0$ must be imposed, such that to select a representative in each equivalence class.

We further can exploit the local phase-uncertainty of the wave-function. The stationary group of the momentum $\mathbf{p}$ is the $SO(2) \cong U(1)$ group, i.e.

$$R_{\mathbf{p}}(\chi)\mathbf{p}R_{\mathbf{p}}^{-1}(\chi) = \mathbf{p}, \qquad (21)$$

where R is a rotation operator and χ is the rotation angle about the wave-vector $\mathbf{p}$. This also reflects the operator identity $\mathbf{p}\cdot\mathbf{l} = 0$, where $\mathbf{l} = \mathbf{r}\times\mathbf{p}$ is the kinematic angular momentum. The eigenfunctions of the rotation operator $-i\partial_\chi$ are phase factors

$$-i\partial_\chi e^{i\Lambda\chi}\big|_{\mathbf{p}} = \Lambda\, e^{i\Lambda\chi}\big|_{\mathbf{p}}, \qquad (22)$$

where Λ is some angular momentum quantum number and $\chi = \chi(\mathbf{p})$. Each vector $\mathbf{v}$ in the space $T_{\mathbf{p}}$ tangential to the momentum can be expanded

$$\mathbf{v} = v_\theta(\mathbf{p})\partial_\theta + v_\varphi(\mathbf{p})\partial_\varphi, \qquad (23)$$

where the angles (θ, φ) specify the orientation of the wave-vector $\mathbf{p}$ in a space-fixed frame. The phase angle χ can be defined by the equation

$$\tan\chi = \frac{v_\theta}{v_\varphi}\bigg|_{\mathbf{p}}, \qquad (24)$$

which locally changes in the interval $0 \le \chi \le 2\pi$. In view of arbitrariness of $\mathbf{v}$, at each point $\mathbf{p}$ of the momentum space, we have the freedom to change locally the rotation angle $\chi(\mathbf{p}) \to \chi(\mathbf{p}) + \alpha(\mathbf{p})$ without affecting physical content. Since phase transformations of the wave-function

$$\psi(\mathbf{p}) \to \psi(\mathbf{p})e^{i\Lambda\chi(\mathbf{p})} \qquad (25)$$

do not change the equation of motion, and no gauge-fixing conditions are imposed, the cyclic angle χ is a redundant gauge degree-of-freedom and the momentum space of the particle looks locally like $S^2 \times S^1$. The phase angle χ, however can affect the quantization of the orbital angular momentum. The changes of the momentum under infinitesimal variation $\mathbf{p} \to \mathbf{p} + d\mathbf{p}$ induce Abelian $U(1)$ background gauge potential one-form $x = d\mathbf{p}\cdot\mathbf{x}(\mathbf{p})$ over the momentum space

$$d\mathbf{p}\cdot\langle\Lambda(\mathbf{p})|i\nabla_{\mathbf{p}}|\Lambda(\mathbf{p})\rangle = d\mathbf{p}\cdot\hat{\varphi}\frac{\Lambda}{p}\cot\theta, \qquad (26)$$

which maps the gradient of the phase of the wave-function, i.e. measures the phase differences between wave-function values at different points. When χ is redefined locally

$$|\Lambda(\mathbf{p})\rangle \to |\Lambda(\mathbf{p})\rangle e^{-if(\mathbf{p})}, \quad \mathbf{x}(\mathbf{p}) \to \mathbf{x}(\mathbf{p}) + \nabla_{\mathbf{p}} f(\mathbf{p}) \qquad (27)$$

the induced displacement field $\mathbf{x}(\mathbf{p})$ transforms as a gauge field as it should, since the one-form $x(\mathbf{v}) = \mathbf{v}\cdot\mathbf{x}$ takes values on vectors in $\mathbf{v} \in T_{\mathbf{p}}$, which are not observable. If the momentum $\mathbf{p}$ is displaced continuously along a closed curve C, the phase-factor $\psi(\chi) = \exp i\Lambda\chi$ satisfies the eigen-value equation $-i\partial_\chi\psi(\chi) = \Lambda\psi(\chi)$ at each point $\mathbf{p}$. When the wave-vector returns to its original direction, the wave-function is multiplied by a Berry's phase-factor [14]

$$\psi(\chi) \to \psi(\chi)\exp(i\oint_C x) = \psi(\chi)\exp i\gamma(C), \qquad (28)$$

which generates a shift of the angle $\chi \to \chi + \gamma(C)/\Lambda$, i.e. a gauge transformation. The gauge-field exhibits Dirac string singularity along the entire z-axis, and can not be defined globally. Singularity-free induced displacement fields can be defined on two overlapping local patches as e.g. [16, 17]

$$\mathbf{x}^N = \frac{\Lambda}{p}\frac{\cos\theta - 1}{\sin\theta}\hat{\varphi}, \quad R_N : 0 \le \theta < (\pi+\varepsilon)/2$$
$$\mathbf{x}^S = \frac{\Lambda}{p}\frac{\cos\theta + 1}{\sin\theta}\hat{\varphi} \quad R_S : (\pi-\varepsilon)/2 < \theta \le \pi \qquad (29)$$

where the displacement field $\mathbf{x}^N$ is regular on the north hemi-sphere R^N, while $\mathbf{x}^S$ is regular on the southern hemi-sphere R^S. Near the equator $R^N \bigcap R^S$, these fields are related by local gauge-transformation

$$\mathbf{x}^S \to \mathbf{x}^S - ie^{-2i\Lambda\varphi}\nabla_{\mathbf{p}}e^{2i\Lambda\varphi} = \mathbf{x}^N. \qquad (30)$$

The induced displacement field is not rotation symmetric, since under rotation $d\mathbf{p} = \mathbf{n}\times\mathbf{p}$ it changes form. Coordinate frame rotations are supplemented by local redefinitions of the phase angle $\chi(\mathbf{p})$, such that rotation non-symmetric terms be compensated, i.e. the following equation is satisfied

$$\mathbf{n}\times\mathbf{x} - \mathbf{n}\times\mathbf{p}\cdot\nabla_{\mathbf{p}}\mathbf{x} = -\nabla_{\mathbf{p}} f(\mathbf{p}) \qquad (31)$$

where $f(\mathbf{p})$ is a compensating phase function. The gauge field does not change form under Galilei boost transformations with parameter $\delta\mathbf{v}$, i.e.

$$G\mathbf{x}(G^{-1}\mathbf{p}) = \mathbf{x}, \tag{32}$$

for $G = I + i\delta\mathbf{v}\cdot\mathbf{r}$. The gauge field leads to rotation symmetric effects through its induced displacement field strength two-form $F = dx = (\partial_i x_j(\mathbf{p}) - \partial_j x_i(\mathbf{p}))dp^i \wedge dp^j$, its dual vector $F_i = \varepsilon_{ijk}F_{jk}$ or magnetic-like field is

$$\mathbf{F} = \nabla_{\mathbf{p}} \times \mathbf{x}(\mathbf{p}) = -\frac{\Lambda}{p^2}\hat{\mathbf{p}}, \tag{33}$$

Further, the kinematic angular momentum $\mathbf{l} = \mathbf{r}\times\mathbf{p}$ of the particle is supplemented by nonkinematic correction

$$\mathbf{l} = -\mathbf{p}\times\mathbf{d} + \frac{\partial W}{\partial \mathbf{n}}, \tag{34}$$

where $W = \Lambda\mathbf{n}\cdot\hat{\mathbf{p}}$ is the generator of local phase transformations, corresponding to phase function $f(\mathbf{p}) = \Lambda\mathbf{n}\cdot\hat{\mathbf{p}} - \mathbf{n}\times\mathbf{p}\cdot\mathbf{x}$ in Eq.(31). The angular momentum $\Lambda\hat{\mathbf{p}}$ is the angular momentum stored in the gauge field. $U(1)$ gauge-invariant Galilei boost generator $\mathbf{d}$ is

$$\mathbf{d} = \mathbf{r} + \mathbf{x}(\mathbf{p}) \tag{35}$$

and $\mathbf{r} = i\nabla_{\mathbf{p}}$ is the noninvariant canonical operator of the position. The operator of the position $\mathbf{d}$ is non-commutative, and satisfies the relations

$$[d_i, d_j] = -i\Lambda\varepsilon_{ijk}\frac{p_k}{p^3}, \quad [d_i, p_j] = i\delta_{ij} \tag{36}$$

that conserve canonical commutation relation between position and momentum. For spin-less particles $\Lambda = 0$, the coordinates commute. It is important however, that the Jacobi identity is not satisfied

$$[[d_1, d_2], d_3] + [[d_2, d_3], d_1] + [[d_3, d_1], d_2] = -4\pi\Lambda\delta^{(3)}(\mathbf{p}) \tag{37}$$

The gauge invariant representation of Galilei boost transformations is based on the operator

$$G(\mathbf{v}) = \exp(i\mathbf{v}\cdot\mathbf{d}), \tag{38}$$

which generates transformation of the wave-function according to

$$G(\mathbf{v})\psi(\mathbf{p}) = \exp(i\mathbf{v}\cdot\mathbf{d})\exp(-i\mathbf{v}\cdot\mathbf{r})\psi(\mathbf{p}-\mathbf{v}). \tag{39}$$

The product of the two exponentials is easily evaluated and given by a line integral

$$\exp(i\mathbf{v}_1\cdot\mathbf{d})\exp(-i\mathbf{v}_1\cdot\mathbf{r}) = \exp\left(i\int_{\mathbf{p}-\mathbf{v}_1}^{\mathbf{p}} d\mathbf{q}\cdot\mathbf{x}(\mathbf{q})\right) \tag{40}$$

connecting the frame $\mathbf{p}-\mathbf{v}_1$ to $\mathbf{p}$. Application of second Galilei transformation $G(\mathbf{v}_2)$, shows that

$$G(\mathbf{v}_1)G(\mathbf{v}_2) = \exp\left[i\Pi(\mathbf{p};\mathbf{v}_1,\mathbf{v}_2)\right]G(\mathbf{v}_1+\mathbf{v}_2), \tag{41}$$

where $\Pi(\mathbf{p};\mathbf{v}_1,\mathbf{v}_2) = \oint_\triangle x = \Lambda\Omega_\triangle$ is the Berry's phase [14], i.e. the solid angle subtended by triangle $\triangle$ formed by the vertices of the wave-vectors $\mathbf{p}$, $\mathbf{p}-\mathbf{v}_1$ and $\mathbf{p}-\mathbf{v}_1-\mathbf{v}_2$, as seen from the rest frame $\mathbf{p} = \mathbf{0}$ of the particle. Therefore the composition law of the Galilei boost transformations is in general non-associative, e.g. [15]. The associativity of the Galilei boost transformations is expressed by the equation

$$[G(\mathbf{v}_1)G(\mathbf{v}_2)]G(\mathbf{v}_3) = G(\mathbf{v}_1)[G(\mathbf{v}_2)G(\mathbf{v}_3)]. \tag{42}$$

Taking into account Eq.(41), the associativity of finite Galilei boost transformations is restored, if and only if the flux $\oint_S F$ of the displacement field strength two-form through a tetrahedron enclosing the wave-vector $\mathbf{p}$ by the three Galilei transformations, is quantizied according to $\Lambda = N/2$. Therefore quantization of the helicity Λ with half-integer numbers is a consequence of associativity of finite Galilei boost transformations. Canonical commutation relations between the components of the $U(1)$ gauge-invariant rotation operator $[l_i, l_j] = i\varepsilon_{ijk}l_k$ hold for $\Lambda = N/2$. The square of the angular momentum operator in Eq.(34) can be written as

$$\mathbf{l}^2 = -\frac{1}{\sin^2\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \right.$$
$$\left. + \left(\frac{\partial}{\partial\varphi} + i\Lambda(1-\cos\theta)\right)^2\right] + \Lambda^2 \tag{43}$$

and the rotation operator about the z-axis is $l_z = -i\partial_\varphi + \Lambda$. Angular momentum eigen-functions are determined by the equations

$$\mathbf{l}^2|lm\Lambda\rangle = l(l+1)|lm\Lambda\rangle, \quad l_z|lm\Lambda\rangle = m|lm\Lambda\rangle, \tag{44}$$

for $l = |\Lambda|, |\Lambda|+1, \ldots$ and $-l \le m \le l$. Wave-functions given by sectional Wu-Yang monopole harmonics

$$Y_{lm\Lambda}(\theta,\varphi) = \langle\theta,\varphi|lm\Lambda\rangle \tag{45}$$

or more explicitly, these are given by means of Jacobi polynomials $P_n^{(\alpha,\beta)}(z)$ as

$$Y_{lm\Lambda}(\theta,\varphi) = N_{lm}(1-z)^{-(\Lambda+m)/2}(1+z)^{-(\Lambda-m)/2}\times$$
$$\times P_{l+m}^{(-\Lambda-m,-\Lambda+m)}(z)e^{i(\Lambda+m)\varphi}, \tag{46}$$

where $z = \cos\theta$ and N_{lm} are normalization constants. Components of the gauge-invariant rotation operator $\mathbf{l}$ satisfy canonical commutation relations $[l_i, l_j] = i\varepsilon_{ijk}l_k$, and therefore are connected to the Wigner's rotation functions by

$$Y_{lm\Lambda}(\theta,\varphi) = D^l_{\Lambda m}(-\varphi,\theta,\varphi) = \langle l\Lambda|e^{-i\varphi l_z}e^{i\theta l_y}e^{i\varphi l_z}|lm\rangle. \tag{47}$$

The sign of Λ, $\mathrm{sign}(\Lambda) = \pm 1$ distinguishes left-handed from right-handed rotations, which commute. The wave-function is χ-independent, single particle states labelled by four quantum numbers

$$|\psi\rangle = |Elm\Lambda\rangle \tag{48}$$

and E is the kinetic energy of the particle. The states with $|\Lambda| = 0, 1, 2 \ldots$ form representation of the rotation group of integer angular momentum. For $\Lambda = 0$, they reduce to the conventional spherical harmonics $Y_{lm}(\hat{\mathbf{p}})$. The states corresponding to half-integer angular momentum $|\Lambda| = 1/2, 3/2, \ldots$ define spinor representations of the rotation group. For instance, a doublet of wave-functions corresponding to $l = \Lambda = 1/2$ is given by means of half angles

$$Y_{\frac{1}{2}\frac{1}{2}\frac{1}{2}}(\theta,\varphi) = -\sin\frac{\theta}{2}e^{i\varphi}, \quad Y_{\frac{1}{2}-\frac{1}{2}\frac{1}{2}}(\theta,\varphi) = \cos\frac{\theta}{2}, \quad (49)$$

on the northern hemi-sphere of the momentum space. Second doublet of wave-functions with $\Lambda = 1/2$ with support on the southern hemi-sphere is obtained by spatial inversion $\theta \to \pi - \theta, \varphi \to \varphi + \pi$. Second group of left-moving helicity eigen-states of $\Lambda = -1/2$ is obtained by complex conjugation of wave-functions of right-handed particle states.

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C. Motion of two free electrons.

The Schrödinger equation of motion for one free electron in presence of identical spectator electron is,

$$\left(\mathbf{p}_1^2 - \lambda\right)\psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = 0, \quad (50)$$

where $\mathbf{p}_1 = -i\nabla_{\mathbf{r}_1}$ is the momentum of the active electron. The interchange of the particles' position vectors and spins $(\mathbf{r}_1\sigma_1) \leftrightarrow (\mathbf{r}_2\sigma_2)$ leads to identical description of the motion of the spectator electron

$$\left(\mathbf{p}_2^2 - \lambda\right)\psi(\mathbf{r}_2\sigma_2, \mathbf{r}_1\sigma_1) = 0. \quad (51)$$

Since the interchange of particles changes only the sign of the wave-function, the comparison of Eq.(50) with Eq.(51) shows that the kinetic energies of the two particles are equal, i.e.

$$\mathbf{p}_1^2|\psi\rangle = \mathbf{p}_2^2|\psi\rangle = 2\lambda|\psi\rangle \quad (52)$$

the particles move such that to conserve identical their de-Brogile wave-lengths $\lambda_{\mathrm{dB}} = 2\pi/\sqrt{2\lambda}$. In addition particles exhibit identical spins s, i.e.

$$\mathbf{s}_1^2|\psi\rangle = \mathbf{s}_2^2|\psi\rangle = s(s+1)|\psi\rangle. \quad (53)$$

The effects of particle interchange do not involve exchanging energy and momentum and can be represented by rotations of unit vectors $\hat{\mathbf{p}}_1$ and $\hat{\mathbf{p}}_2$ along with rotations of half-integer spins, since magnitudes of momenta $p_1 = p_2 = \sqrt{2\lambda}$ and spins s are not relevant for the description of the effect of particle interchange, i.e. if for instance the momenta are simultaneously scaled according to $\mathbf{p}_1 \to e^{\theta}\mathbf{p}_1$ and $\mathbf{p}_2 \to e^{\theta}\mathbf{p}_2$, then the constraint equation remains unchanged. The equation of motion for the active electron is invariant under bi-local phase change of the wave-function in momentum space

$$\psi(\mathbf{p}_1, \mathbf{p}_2) \to \psi(\mathbf{p}_1, \mathbf{p}_2)e^{if(\mathbf{p}_1,\mathbf{p}_2)} \quad (54)$$

and is invariant under s-wave transformation

$$\psi(\mathbf{p}_1, \mathbf{p}_2) \to \psi(\mathbf{p}_1, \mathbf{p}_2) + \delta(p_1 - k)c(\mathbf{p}_2), \quad (55)$$

where $c(\mathbf{p}_2)$ is an arbitrary function of the spectator momentum. For comparison, the conventional two-particle Schrödinger equation

$$(\mathbf{p}_1^2 + \mathbf{p}_2^2 - 2E)\psi(\mathbf{p}_1, \mathbf{p}_2) = 0 \quad (56)$$

is invariant under bi-local phase transformation, and similar s-wave transformation

$$\psi(\mathbf{p}_1, \mathbf{p}_2) \to \psi(\mathbf{p}_1, \mathbf{p}_2) + c\delta(p_1 - k)\delta(p_2 - k). \quad (57)$$

We further could separate the orbital from the spin variables, by demanding that the total wave-function be an eigen-function of total spin $\mathbf{S} = \mathbf{s}_1 + \mathbf{s}_2$, together with its projection M onto a space-fixed unit-vector $\hat{\mathbf{P}}$, i.e.

$$\mathbf{S}^2|\psi_S\rangle = S(S+1)|\psi_S\rangle, \quad \hat{\mathbf{P}}\cdot\mathbf{S}|\psi_S\rangle = M|\psi_S\rangle \quad (58)$$

and the wave-function is

$$\psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = \psi_S(\mathbf{r}_1, \mathbf{r}_2)C^{SM}_{s\sigma_1,s\sigma_2}. \quad (59)$$

The Clebcsh-Gordan coefficient changes under interchange of spins $\sigma_1 \leftrightarrow \sigma_2$ as

$$C^{SM}_{s\sigma_1 s\sigma_2} = (-1)^{2s-S}C^{SM}_{s\sigma_1,s\sigma_2}. \quad (60)$$

and implies that under interchange of spatial coordinates

$$\psi_S(\mathbf{r}_1, \mathbf{r}_2) = (-1)^S\psi_S(\mathbf{r}_2, \mathbf{r}_1), \quad (61)$$

the wave-function is multiplied by the phase-factor $(-1)^S$. We further change the individual coordinates to collective coordinates for the relative $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and center-of-mass motion $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$. The momenta, which are conjugate to these coordinates are $\mathbf{p} = -i\nabla_{\mathbf{r}}$ and $\mathbf{P} = -i\nabla_{\mathbf{R}}$, respectively. The equation of motion reads

$$\left(\frac{1}{2}\mathbf{p}^2 + \frac{1}{2}\mathbf{p}\cdot\mathbf{P} + \frac{1}{8}\mathbf{P}^2 - \lambda\right)\psi_S(\mathbf{R}, \mathbf{r}) = 0, \quad (62)$$

and the boundary condition of Eq.(3) now reads

$$\psi_S(\mathbf{R}, \mathbf{r}) = (-1)^S\psi_S(\mathbf{R}, -\mathbf{r}), \quad (63)$$

The inter-change of spatial coordinates $\mathbf{r} \to -\mathbf{r}$ in Eq.(62) leads to the equation of motion for the spectator electron

$$\left(\frac{1}{2}\mathbf{p}^2 - \frac{1}{2}\mathbf{p}\cdot\mathbf{P} + \frac{1}{8}\mathbf{P}^2 - \lambda\right)\psi_S(\mathbf{R}, \mathbf{r}) = 0, \quad (64)$$

Since Eq.(62) and Eq.(64) are satisfied simultaneously, we have single first-class constraint on the dynamics

$$\mathbf{P}\cdot\mathbf{p}|\psi_S\rangle = 0, \tag{65}$$

that particles share the kinetic energy in equal way, and therefore can not be distinguished. The presence of spectator particle is non-trivial, since it constraints the wave-function of the two-particle state. Hamiltonians in Eq.(62) and Eq.(64) together with the constraint of Eq.(65) are translation and rotation invariant. We further constraint the wave-function to be an eigen-function of the conserved momentum $\mathbf{P}$ of the center-of-mass motion

$$\psi_S(\mathbf{R},\mathbf{r}) = e^{i\mathbf{P}\cdot\mathbf{R}}\psi_{S,\mathbf{P}}(\mathbf{r}), \tag{66}$$

and re-write the equation for the relative motion as

$$\left(\mathbf{p}^2 - k^2\right)\psi_{S,\mathbf{P}}(\mathbf{r}) = 0, \tag{67}$$

where $k^2 = 2\lambda - P^2/4$. The relative wave-function is subject to constraint for anti-symmetry

$$\psi_{S,\mathbf{P}}(\mathbf{r}) = (-1)^S\psi_{S,\mathbf{P}}(-\mathbf{r}). \tag{68}$$

By neglecting effects of spin, the solution of Eq.(64) can be written as

$$\psi_{\mathbf{P}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}e^{if_{\mathbf{P}}(\mathbf{r})}, \tag{69}$$

i.e. the phase of the unconstrained Schrödinger's wave-function is re-defined locally by the constraint for equal sharing of kinetic energy. Since the particles are free, the phase-function $f_{\mathbf{P}}(\mathbf{r})$ is a linear function of the relative coordinate $\mathbf{r}$, i.e. $f(\mathbf{r}) = \mathbf{A_P}\cdot\mathbf{r}$, where $\mathbf{A_P}$ is a constant vector. The non-trivial solution for the compensating vector is $\mathbf{A_P} = -(\mathbf{k}\cdot\hat{\mathbf{P}})\hat{\mathbf{P}}$. The wave-function is therefore given by

$$\psi_{\mathbf{P}}(\mathbf{r}) = e^{i[\mathbf{k}\cdot\mathbf{r}-(\mathbf{k}\cdot\hat{\mathbf{P}})(\mathbf{r}\cdot\hat{\mathbf{P}})]}, \tag{70}$$

and the kinetic energy of relative motion is $\varepsilon = \mathbf{k}^2 - (\mathbf{k}\cdot\hat{\mathbf{P}})^2$, indicating that the component of the relative momentum $\mathbf{k}$ on the direction of propagation $\hat{\mathbf{P}}$ is redundant. The kinematic constraint for equal sharing of kinetic energy annihilates the wave-function

$$\delta_\varepsilon\psi_{\mathbf{P}}(\mathbf{r}) = \varepsilon\mathbf{P}\cdot\mathbf{p}\psi_{\mathbf{P}}(\mathbf{r}) = 0 \tag{71}$$

where ε is an uniform gauge parameter, i.e. under the transformation

$$\psi_{\mathbf{P}}(\mathbf{r}) \to \psi_{\mathbf{P}}(\mathbf{r}) + \delta_\varepsilon\psi_{\mathbf{P}}(\mathbf{r}) \approx \psi(\mathbf{r}+\varepsilon\mathbf{P}) \tag{72}$$

the two-electron wave-function remains unchanged. Furthermore the uniform parameter ε can be "gauged" into a function $\varepsilon = \varepsilon(\mathbf{r})$. The particle identity constraint is a generator of canonical transformations of the variables in the dynamic system, the relative coordinate is gauge-dependent and changes as

$$\delta_\varepsilon\mathbf{r}|\psi_{\mathbf{P}}\rangle = -i\varepsilon[\mathbf{r},\mathbf{P}\cdot\mathbf{p}]|\psi_{\mathbf{P}}\rangle = \varepsilon\mathbf{P}|\psi_{\mathbf{P}}\rangle, \tag{73}$$

i.e. acquires a longitudinal correction. The property of sign-change of the vector $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ inter-connecting the particles under interchange is not unique, since the physically equivalent position vector $\mathbf{r}+\varepsilon\mathbf{P} \to -\mathbf{r}+\varepsilon\mathbf{P}$ does not change sign, unless the transformation $\mathbf{r}_1 \leftrightarrow \mathbf{r}_2$ is supplemented by reversal of the sign of $\mathbf{P}$. However, the momentum of relative motion is unchanged, i.e. $\delta_\varepsilon\mathbf{p}|\psi_{\mathbf{P}}\rangle = 0$, i.e. the interchange of momenta $\mathbf{p}\to-\mathbf{p}$ is gauge-invariant transformation. The relative angular momentum $\mathbf{l} = \mathbf{r}\times\mathbf{p}$ is gauge-dependent

$$\delta_\varepsilon(\mathbf{r}\times\mathbf{p})|\psi_{\mathbf{P}}\rangle = \varepsilon\mathbf{P}\times\mathbf{p}|\psi_{\mathbf{P}}\rangle \neq 0, \tag{74}$$

i.e. $\mathbf{l}\sim\mathbf{l}+\mathbf{P}\times\mathbf{p}$ are equivalent as operators and can be identified, in the same way $\mathbf{L} = \mathbf{R}\times\mathbf{P}\sim\mathbf{L}+\mathbf{p}\times\mathbf{P}$ can be identified. The total angular momentum $\mathbf{J} = \mathbf{L}+\mathbf{l}+\mathbf{S}$ is gauge-invariant. If the position vector interconnecting the particles is resolved as

$$\mathbf{r} = \mathbf{r}_\perp + \mathbf{r}_{||}, \tag{75}$$

where $\mathbf{r}_{||} = \hat{\mathbf{P}}(\hat{\mathbf{P}}\cdot\mathbf{r})$ is the projection onto the propagation wave-vector, while $\mathbf{r}_\perp$ is the rejection, then the gauge invariance of the wave-function is expressed by its independence on the projection $\mathbf{r}_{||}$ and the rejection coordinate $\mathbf{r}_\perp$ is gauge-invariant coordinate.

To take into account more accurately the effect of spin S, the operator of the constraint is resolved

$$\mathbf{P}\cdot\mathbf{p} = P(p_x\sin\Theta\cos\Phi + p_y\sin\Theta\sin\Phi + p_z\cos\Theta), \tag{76}$$

where (P,Θ,Φ) are the spherical coordinates of the propagation wave-vector. The inter-particle position vector is further resolved in a local basis specified by the propagation wave-vector $\hat{\mathbf{P}}$ as

$$\mathbf{r} = r_P\hat{e}_{\mathbf{P}} + r_\Theta\hat{e}_\Theta + r_\Phi\hat{e}_\Phi. \tag{77}$$

The rotation matrix which gives the change of coordinates is

$$\begin{pmatrix} r_P \\ r_\Theta \\ r_\Phi \end{pmatrix} = \begin{pmatrix} \sin\Theta\cos\Phi & \sin\Theta\sin\Phi & \cos\Theta \\ \cos\Theta\cos\Phi & \cos\Theta\sin\Phi & -\sin\Theta \\ -\sin\Phi & \cos\Phi & 0 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} \tag{78}$$

Similarly the momentum of relative motion is expanded over this basis

$$\mathbf{p} = p_P\hat{e}_{\mathbf{P}} + p_\Theta\hat{e}_\Theta + p_\Phi\hat{e}_\Phi \tag{79}$$

At each point $\mathbf{P}$, cylindrical coordinates are introduced

$$\rho = \sqrt{r_\Theta^2 + r_\Phi^2}, \quad \tan\varphi = \frac{r_\Phi}{r_\Theta}, \quad z = r_P \tag{80}$$

The subsidiary condition for equal sharing of kinetic energy takes simple form

$$\partial_z\psi_{\mathbf{P},S}(\rho,\varphi,z) = 0, \tag{81}$$

i.e. wave-function is independent on the longitudinal coordinate z, and is an eigen-function of the operator of the

momentum $p_z = p_P$ with eigenvalue $k_z = k_P = 0$. For each fixed propagation wave-vector $\mathbf{P}$, the wave-function satisfies the equation

$$\left(\partial_\rho^2 + \frac{1}{\rho}\partial_\rho + \frac{1}{\rho^2}\partial_\varphi^2 + k^2\right)\psi_{\mathbf{P},S}(\rho,\varphi) = 0, \tag{82}$$

and $E = k^2$ is the kinetic energy of relative motion. Under π-re-definition of the fiber angle φ, the particles interchange, and their wave changes according to

$$\psi_{\mathbf{P},S}(\rho,\varphi) = e^{iS\pi}\psi_{\mathbf{P},S}(\rho,\varphi+\pi). \tag{83}$$

The solution of Eq.(82) is separable $R(\rho)\phi(\varphi)$ in cylindrical coordinates, and periodic Bloch-type boundary condition in Eq.(83) fixes the solution as

$$\psi_{\mathbf{P},S}(\rho,\varphi,\sigma,\sigma') = J_\Lambda(k\rho)e^{i\Lambda\varphi}C^{SM}_{s\sigma,s\sigma'} \tag{84}$$

where $\Lambda = S\mathrm{mod}(2\hbar)$ is the helicity, which is analogue of a Bloch quasi-angular momentum, $J_\Lambda(z)$ are the Bessel functions of integer order and π is a characteristic angular inter-change period. The sign of Λ determines left or right helicity eigen-states. The inter-change of particles $\mathbf{r} \to -\mathbf{r}$ can be expressed by

$$\psi_{\mathbf{P}}(\varphi+\pi,\sigma',\sigma) = e^{i\pi S}\psi_{\mathbf{P}}(\varphi,\sigma',\sigma) = (-1)^{2s}\psi_{\mathbf{P}}(\varphi,\sigma,\sigma'). \tag{85}$$

where we have used the symmetry property of the Clebsch-Gordan coefficient in Eq.(60). Eq.(85) is only a consequence of the solution of the equations of motion, i.e. if we project the state vector on exchanged configurations $\langle\varphi+\pi,\sigma',\sigma|\psi\rangle = (-1)^{2s}\langle\varphi,\sigma,\sigma'|\psi\rangle$, the multiplicative particle-statistics phase-factor appears automatically. Therefore, the particle inter-change is a gauge transformation of the fiber angle $\varphi \to \varphi+\pi$, which partially compensates the effect of rotation of the phase of the spin wave-function. The "local"-type quantization of Λ by Bloch type boundary condition, is inappropriate, since the phases of wave-functions evaluated at different points can not be compared, which reflects the uncertainty of the phase of the momentum space wave-function.

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The effect of particle identity is shown to entail reduction in the number of the initial six orbital degrees of freedom to five.

D. Two Coulombically interacting electrons in absence of external forces

We consider the problem for the Coulomb scattering of the two particles, when there is no source of external forces. Furthermore, the spin constraints are represented very approximately by Bloch-type boundary condition. Since the Coulombic interaction r_{12}^{-1} is invariant under inter-change of particles, then nothing principal changes as compared to the case of motion of free electrons. The Hamiltonian of the active electron is

$$h_{\mathbf{r}_1} = -\frac{1}{2}\nabla^2_{\mathbf{r}_1} + g r_{12}^{-1}, \tag{86}$$

By inter-changing the coordinates $\mathbf{r}_1 \leftrightarrow \mathbf{r}_2$, we obtain the Hamiltonian for the motion of the spectator particle

$$h_{\mathbf{r}_2} = -\frac{1}{2}\nabla^2_{\mathbf{r}_2} + g r_{21}^{-1}, \tag{87}$$

where $g = 1/2$. Using Eq.(3) that the fermion wave-function only changes sign upon inter-change of particles, we obtain that

$$h_{\mathbf{r}_1}\psi(\mathbf{r}_1,\mathbf{r}_2) = h_{\mathbf{r}_2}\psi(\mathbf{r}_1,\mathbf{r}_2) = \lambda\psi(\mathbf{r}_1,\mathbf{r}_2), \tag{88}$$

i.e. the particles are precisely identical, since Hamiltonians $h_{\mathbf{r}_1}$ and $h_{\mathbf{r}_2}$ exhibit common eigenvalue λ. Therefore, equations of motion are consistent only if one-particle Hamiltonians commute with each other, i.e. $[h(1),h(2)]|\psi\rangle = 0$, which leads to a consistency condition

$$(\mathbf{F}_{12}\cdot\mathbf{p}_1 - \mathbf{F}_{21}\cdot\mathbf{p}_2)|\psi\rangle = 0, \tag{89}$$

where

$$\mathbf{F}_{12} = \frac{\mathbf{r}_{12}}{r_{12}^3} = -\mathbf{F}_{21} \tag{90}$$

is the repulsive Coulomb force of interaction between the two particles. Eq.(89) shows that electrons move such that to screen (compensate) the excess Coulombic force in the direction of the total momentum $\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$. This result has simple classical analogue, since the above equation reads

$$\mathbf{p}_1\cdot\dot{\mathbf{p}}_1 - \mathbf{p}_2\cdot\dot{\mathbf{p}}_2 = 0, \tag{91}$$

and the difference of the kinetic energies of the two particles is a constant of motion

$$\frac{d}{dt}(\mathbf{p}_1^2 - \mathbf{p}_2^2) = 0. \tag{92}$$

When this difference is vanishing, the particles are precisely identical, otherwise they can be distinguished trivially. Furthermore, if the active electron at point $\mathbf{r}_1$ changes its momentum due to the Coulomb force of his partner positioned at $\mathbf{r}_2$, the spectator particle changes its momentum in strictly proportional way, such that the excess force in the direction of the motion of the center-of-mass $\mathbf{P}$ is compensated. The supplementary condition for screening in Eq.(89) of the mutual excess Coulomb forces can be written more simply as

$$\mathbf{r}_{12}\cdot(\nabla_1 + \nabla_2)|\psi\rangle = 0. \tag{93}$$

By means of Eq.(88), we also have that $[h(1)-h(2)]|\psi\rangle = 0$, which is a constraint for equal sharing of kinetic energy by the particles, i.e.

$$[\mathbf{p}_1^2 - \mathbf{p}_2^2]|\psi\rangle = 0. \tag{94}$$

The constraint for screening of the repulsive inter-particle Columbic force can be viewed as a gauge-fixing condition for the invariance generated by the constraint of equilibration of the de-Brogile wave-lengths $\mathbf{p}_1^2 = \mathbf{p}_2^2$. Reintroducing the collective coordinates for relative $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and center-of-mass motion $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, with the corresponding momenta $\mathbf{p} = -i\nabla_{\mathbf{r}}$ and $\mathbf{P} = -i\nabla_{\mathbf{R}}$. Further, the center-of-mass motion is uniform and we impose explicitly three additional constraints for the conservation of the momentum of center-of-mass $\mathbf{P} = (P_x, P_y, P_z)$ motion

$$-i\nabla_{\mathbf{R}}\langle\mathbf{R}|\psi\rangle = \mathbf{P}\langle\mathbf{R}|\psi\rangle, \tag{95}$$

i.e. the two-electron state is an eigen-state characterized by the momentum $\mathbf{P}$, i.e.

$$\psi = e^{i\mathbf{P}\cdot\mathbf{R}}\psi_{\mathbf{P}}(\mathbf{r}). \tag{96}$$

By separating the center-of-mass motion, the Hamiltonian for the relative motion of the two particles becomes

$$H_{rel} = \mathbf{p}^2 + |\mathbf{r}|^{-1}, \tag{97}$$

subject to the supplementary condition for screening $\hat{\mathbf{P}}\cdot\mathbf{r}|\psi_{\mathbf{P},S}\rangle = 0$ and for equal sharing of kinetic energy

$$\hat{\mathbf{P}}\cdot\mathbf{p}|\psi_{\mathbf{P},S}\rangle = 0, \tag{98}$$

and $\hat{\mathbf{P}}$ is a unit vector in the direction of propagation of the center-of-mass motion. In Cartesian coordinates $\mathbf{r} = (r_P, r_\theta, r_\Phi)$ with z-axis parallel to the propagation wave-vector, the pair of supplementary conditions become

$$r_P\langle\mathbf{r}|\psi_{\mathbf{P},S}\rangle = 0, \quad \frac{1}{i}\frac{\partial}{\partial r_P}\langle\mathbf{r}|\psi_{\mathbf{P},S}\rangle = 0, \tag{99}$$

which is a pair of second-class constraints, that show that the longitudinal relative coordinate r_P is locally redundant. The reduced Hamiltonian for the planar orbital motion of the internal degrees-of-freedom simplifies as

$$H_{rel} = p_\Phi^2 + p_\Theta^2 + \frac{1}{\sqrt{r_\Theta^2 + r_\Phi^2}}, \tag{100}$$

The wave-function is subject to the boundary condition

$$\psi_{S,\mathbf{P}}(r_\Theta, r_\Phi) = (-1)^S\psi_{S,\mathbf{P}}(-r_\Theta, -r_\Phi). \tag{101}$$

Introducing the cylindrical coordinates $r_\Theta = \rho\cos\varphi$ and $r_\Phi = \rho\sin\varphi$, the Hamiltonian reads

$$H_{rel} = \left(-\partial_\rho^2 - \frac{1}{\rho}\partial_\rho - \frac{1}{\rho^2}\partial_\varphi^2\right) + \frac{1}{\rho} \tag{102}$$

To comply with scattering state boundary conditions, we specify the orbital collision plane to be formed by the incident wave-vector $\mathbf{k}_i$ and the wave-vector $\mathbf{k}_f$ of the out-going scattered wave and therefore $\hat{\mathbf{P}} = \mathbf{k}_i \times \mathbf{k}_f$ specifies the orientation of the orbital collision plane, which is otherwise arbitrary. We impose planar two-dimensional boundary condition for scattering states as

$$\psi^{(+)}(\mathbf{r}) \approx \psi^{\text{inc}}_{\mathbf{k}_i}(\mathbf{r}) + f_S(k,\varphi)\frac{\mathcal{F}^{(+)}(k\rho)}{\sqrt{\rho}}, \quad \rho\to\infty \tag{103}$$

where ψ^{inc} is the incident Bloch wave, which is superimposed on out-going scattered Bloch wave $\mathcal{F}^{(+)}$ of amplitude $f(\varphi)$. The planar Bloch wave-functions of electronic states exhibit partial wave-expansion as

$$\psi_{S,\hat{\mathbf{P}}}(\rho,\varphi) = e^{iS\varphi}\sum_n e^{2in\varphi}\psi^{(+)}_{2n+S}(k\rho). \tag{104}$$

Similarly, the scattering amplitude exhibits Bloch representation

$$f_S(k,\varphi) = e^{iS\varphi}\sum_n e^{2in\varphi}f_{2n+S}(k), \tag{105}$$

and satisfies

$$f_S(k,\varphi) = (-1)^S f_S(k,\varphi+\pi), \tag{106}$$

i.e. it is symmetric for scattering in a spin-singlet and anti-symmetric otherwise. Instead for the physical wave-function $\psi^{(+)}(k\rho)$, we solve this equation for the regular wave-function $R(k\rho)$, which is subject to the boundary condition that

$$\lim_{\rho\to 0}\rho^{-|\Lambda|}R_{|\Lambda|}(\rho) = 1. \tag{107}$$

and satisfies the equation

$$\frac{d^2}{d\rho^2}R_\Lambda(\rho) + \frac{1}{\rho}\frac{d}{d\rho}R_\Lambda(\rho) + \left(k^2 - \frac{1}{\rho} - \frac{\Lambda^2}{\rho^2}\right)R_\Lambda(\rho) = 0, \tag{108}$$

where $\Lambda = S \bmod 2\hbar$ is the helicity, $k = \sqrt{2(\lambda - P^2/8)}$ and the solution depends only on $|\Lambda|$, and we further take $\Lambda \geq 0$, which is equivalent to take $n \geq 0$ and consider right-handed electronic states. Making the substitution $R_\Lambda = u_\Lambda/\sqrt{\rho}$ in Eq.(108), we obtain the Whittaker's equation

$$\frac{d^2}{dz^2}u_\Lambda(z) + \left(-\frac{1}{4} + \frac{\eta}{z} + \frac{1/4 - \Lambda^2}{z^2}\right)u_\Lambda(z) = 0, \tag{109}$$

where $z = -2ik\rho$ and $\eta = -i/2k$. The general solution of the Whittaker's equation is

$$u_\Lambda(z) = A_\Lambda W_{\eta,\Lambda}(z) + B_\Lambda W_{-\eta,\Lambda}(-z), \tag{110}$$

where A_Λ and B_Λ are integration constants and $W_{\pm\eta,\Lambda}(\pm z)$ are the two linearly independent Whittaker's functions of second kind. The unknown integration constants can be obtained from the boundary condition for the regular solution Eq.(107). The asymptotic of the Whittaker's functions [19], when $|z|\to\infty$,

$$W_{\eta,\Lambda}(z) \to z^\eta e^{-z/2}, \tag{111}$$

gives the asymptotic of the scattering-state wave-function

$$u_\Lambda(z) \approx e^{\pi/2k}\Big[A_\Lambda e^{i(k\rho-\log 2k\rho/k)}+ + B_\Lambda e^{-i(k\rho-\log 2k\rho/k)}\Big], \quad \rho\to\infty, \tag{112}$$

as linear combination of irregular Jost solutions, specified by the boundary conditions

$$\lim_{\rho\to\infty} e^{\mp i[k\rho-\log 2k\rho/k]}\mathcal{F}^{(\pm)}(k\rho)=1, \tag{113}$$

and describe polar Coulomb waves outgoing from [with sign (+)] or incoming [with (−) sign] towards the origin $\rho=0$. The Jost solutions and Whittaker's functions are identical up to multiplicative Λ-independent constant, more specifically the relation is given by

$$\mathcal{F}^{(\pm)}(k\rho)=e^{\pi/2k}W_{\pm\eta,\Lambda}(\pm z), \tag{114}$$

and these functions can be identified by Λ-independent re-definition of integration constants

$$A\to Ae^{\pi/2k}=\mathrm{f}^{(-)}(k), \quad B\to Be^{\pi/2k}=-\mathrm{f}^{(+)}(k), \tag{115}$$

The wave-function can be re-written as linear combination of the two Jost solutions

$$u(\rho)=\frac{1}{w(k)}[\mathrm{f}^{(-)}(k)\mathcal{F}^{(+)}(k\rho)-\mathrm{f}^{(+)}(k)\mathcal{F}^{(-)}(k\rho)], \tag{116}$$

where $w(k)=W[\mathcal{F}^{(-)},\mathcal{F}^{(+)}]=2ik$ is the Wronskian of the two Jost solutions, i.e. $W[f,g]=fg'-f'g$ and prime denotes radial derivative. The integration constants $\mathrm{f}^{(\pm)}$ are the Jost functions, which are given by the Wronskians

$$\mathrm{f}^{(\pm)}(k)=W[\mathcal{F}^{(\pm)},u], \tag{117}$$

which we evaluate at the origin $\rho=0$. By using the asymptotic of the irregular solutions near the origin

$$\lim_{|z|\to 0} z^{\Lambda-1/2}W_{\eta,\Lambda}(z)=\frac{\Gamma(2\Lambda)}{\Gamma(\Lambda+i/2k+1/2)} \tag{118}$$

and evaluating Wronskians with the help of the boundary condition in Eq.(107), we obtain Jost functions as

$$\mathrm{f}^{(\pm)}(k)=e^{\pi/2k}(\mp 2ik)^{1/2-\Lambda}\frac{\Gamma(2\Lambda+1)}{\Gamma(\Lambda\pm i/2k+1/2)}, \tag{119}$$

where $\Gamma(z)$ is the Euler's gamma function. Then the asymptotic scattering-state wave-function $\rho\to\infty$ is given by

$$u_\Lambda(\rho)\approx\frac{e^{\pi/2k}(2k)^{-1/2-\Lambda}\Gamma(2\Lambda+1)}{|\Gamma(\Lambda+1/2+i/2k)|}e^{i\delta_\Lambda}\times \times\sin\left(k\rho-\frac{1}{k}\log 2k\rho-\frac{\pi\Lambda}{2}-\frac{\pi}{4}+\delta_\Lambda\right), \tag{120}$$

where δ_Λ are elastic scattering phase shifts

$$\delta_\Lambda(k)=\arg\Gamma(\Lambda+1/2+i/2k), \tag{121}$$

relative to the asymptotic of the non-interacting Bessel's function $J_\Lambda(k\rho)$,

$$J_\Lambda(z)\approx\sqrt{\frac{2}{\pi z}}\cos\left(z-\frac{\pi\Lambda}{2}-\frac{\pi}{4}\right). \tag{122}$$

The Coulombic S-matrix is given by the factor of the Jost functions

$$S_\Lambda(k)=\frac{\mathrm{f}^{(-)}(k)}{\mathrm{f}^{(+)}(k)}=e^{2i\delta_\Lambda(k)}. \tag{123}$$

The physical wave-function differs from the regular wave-function be a normalization constant determined from the Jost function, i.e.

$$\psi^{(+)}_\Lambda(k\rho)=N_\Lambda(k)\frac{u_\Lambda(k\rho)}{\sqrt{2k\rho}}, \tag{124}$$

and therefore

$$N_\Lambda(k)=e^{-\pi/2k}(2k)^\Lambda\frac{\Gamma(\Lambda+1/2+i/2k)}{(2\Lambda)!}. \tag{125}$$

As a result, we obtain the partial-wave scattering amplitudes f_Λ as

$$f_\Lambda(k)=\frac{e^{-i\pi/4}}{\sqrt{2\pi k}}[e^{2i\delta_\Lambda(k)}-1]. \tag{126}$$

We next evaluate a differential cross-section for scattering in a given line segment in the collision plane as

$$dP_\varphi=|f(\varphi)|^2d\varphi. \tag{127}$$

To evaluate outgoing scattered probability flux through a solid angle $d\Omega$, we vary the wave-vector $\mathbf{k}_f$, such that the unit vector $\mathbf{k}_i\times\mathbf{k}_f$ normal to the scattering plane rotates on angle α about the axis of incidence $\mathbf{k}_i$, and a generated linear flux is

$$dP_\alpha=|f(\varphi)|^2(\sin\varphi d\alpha). \tag{128}$$

Therefore elastic scattering cross-section is given by

$$d\sigma=dP_\varphi dP_\alpha=|f(\varphi)|^4d\Omega, \tag{129}$$

where $d\Omega=\sin\varphi d\varphi d\alpha$ is the solid angle of observation in the space-fixed reference frame. The differential cross-section is given by

$$\frac{d\sigma}{d\hat{\mathbf{k}}_f}=\frac{d\sigma(\hat{\mathbf{k}}_f\leftarrow\hat{\mathbf{k}}_i)}{d\Omega}=|f(k,\varphi)|^4, \tag{130}$$

and exhibits characteristic dependence on the fourth power of the amplitude.

E. Quasi-classical approximation

In quasi-classical approximation, the two-electron wave-function is a phase-factor

$$\psi = e^{iS}, \tag{131}$$

expanding the phase $S = S_0 + \hbar S_1 + \ldots$, to zero'th order in the Planck's constant, we obtain the equation of motion for the active electron as

$$\frac{1}{2}[\nabla_{\mathbf{r}_1} S_0(\mathbf{r}_1, \mathbf{r}_2)]^2 + g|\mathbf{r}_1 - \mathbf{r}_2|^{-1} = \lambda, \tag{132}$$

together with the constraint for particle identity

$$[\nabla_{\mathbf{r}_1} S_0(\mathbf{r}_1, \mathbf{r}_2)]^2 = [\nabla_{\mathbf{r}_2} S_0(\mathbf{r}_1, \mathbf{r}_2)]^2. \tag{133}$$

The quasi-classical Coulmbic action has the form

$$S_0(\mathbf{r}, \mathbf{R}) = \mathbf{P} \cdot \mathbf{R} + \sigma_{\mathbf{P}}(\mathbf{r}_\perp), \tag{134}$$

where the action for the relative motion satisfies the equation

$$[\nabla_\perp \sigma_{\mathbf{P}}]^2 + \frac{1}{r_\perp} = k^2, \tag{135}$$

where $1/r_\perp$ is the screened planar Coulomb potential. Re-introducing plane polar coordinates $\mathbf{r}_\perp = (\rho, \varphi)$ to describe a collision, the quasi-classical equation reduces exactly to the Hamilton-Jacobi equation of the planar Kepler problem

$$[\partial_\rho \sigma]^2 + \frac{1}{\rho^2}[\partial_\varphi \sigma]^2 + \frac{1}{\rho} = k^2. \tag{136}$$

and has solutions

$$\sigma = \pm \Lambda \varphi + \sigma_\Lambda(\rho), \tag{137}$$

where Λ labels the helicity. The quasi-classical approximation holds if $\Lambda \gg 1$, and therefore we will neglect effects of quantization of Λ. The planar Kepler problem exhibits dynamical symmetry (e.g. [20, 21]), due to the conservation of the planar Laplace-Runge-Lenz vector, which is given by (we use the classical expression, which does not involve hermitian symmetrization)

$$\mathbf{A} = \mathbf{p} \times \mathbf{l} + \hat{\mathbf{r}}, \tag{138}$$

where $\mathbf{l} = \mathbf{r} \times \mathbf{p}$ is the relative angular momentum, $\mathbf{p} = \nabla_{\mathbf{r}} \sigma(\mathbf{r}_\perp)$ is the relative quasi-classical momentum and $\mathbf{A} \cdot \mathbf{l} = 0$. The classical trajectories of relative motion of the two-electrons can be obtained from

$$\mathbf{r} \cdot \mathbf{A} = \rho A \cos\varphi = \Lambda^2 + \rho \tag{139}$$

which leads to the conical section equation, specifying unbound hyperbolic Kepler orbits

$$\frac{p}{\rho} = -1 + e\cos\varphi, \tag{140}$$

with parameter $p = \Lambda^2$ and eccentricity $e = A = \sqrt{1 + k^2\Lambda^2} > 1$, and the point of closest approach on the trajectory ($\varphi = 0$) is $\rho_{min} = p/(e-1)$. The cross-section for elastic scattering can be derived from the conservation of the Runge-Lenz vector. In a reference frame, where the center-of-mass motion is at rest $\mathbf{P} = \mathbf{0}$, we choose the direction of incidence $\hat{\mathbf{k}}_i$ be the negative half of the x-axis of the laboratory frame, the asymptotic momentum of relative motion is $\mathbf{k}_i = k\hat{e}_x$, the angular momentum of relative motion corresponding to this choice is $\Lambda = xp_y - yp_x = -bk$, where b is the impact parameter, and $\hat{e}_y$ is a unit vector in the plane of the orbit. The Laplace-Runge-Lenz vector prior to the collision is given by

$$\mathbf{A}_{in} = -\hat{e}_x + bk^2\hat{e}_y, \tag{141}$$

and similarly after the collision

$$\mathbf{A}_{out} = \hat{e}_{out} + bk^2\hat{\mathbf{n}}_{out}, \tag{142}$$

where $\hat{e}_{out} = \hat{\mathbf{r}}_\perp$ is a unit vector specifying the outgoing direction of the scattered particles, $\hat{\mathbf{n}}_{out} = \hat{\mathbf{P}} \times \hat{e}_{out}$ is a unit-vector in the collision plane, and $\hat{\mathbf{P}}$ is the unit vector normal to the plane of the orbit. By projecting the conserved Runge-Lenz vector onto the direction of incidence, i.e.

$$\hat{e}_x \cdot \mathbf{A}_{in} = \hat{e}_x \cdot \mathbf{A}_{out}, \tag{143}$$

we obtain that

$$-1 = \cos\chi - bk^2 \sin\chi, \tag{144}$$

where χ is a rotation angle, $\cos\chi = \hat{e}_x \cdot \hat{e}_{out}$. From Eq.(144) we obtain the relation $b = b(\chi)$ between the deflection angle and the impact parameter as

$$b = \frac{1}{k^2 \tan\chi/2}. \tag{145}$$

Differentiating with respect to χ, we obtain

$$\left|\frac{db}{d\chi}\right| = \frac{1}{2k^2 \sin^2\chi/2}. \tag{146}$$

The classical differential scattering cross-section is given by $d\sigma = 2\pi b db$, and by using that $d\Omega = 2\pi \sin\chi d\chi$, together with Eq.(145) and Eq.(146) we obtain the Rutherford formula for the cross-section

$$\frac{d\sigma}{d\Omega} = \frac{1}{4k^4 \sin^4\chi/2}. \tag{147}$$

Taking into account reflection symmetry $\chi \to \pi - \chi$, i.e. that we can not distinguish between forward and backward scattering when the particles are identical, we obtain that

$$\frac{d\sigma(\pi - \chi)}{d\Omega} = \frac{1}{4k^4 \cos^4\chi/2} \tag{148}$$

The total cross-section for elastic scattering is obtained by the sum of the two contributions

$$\frac{d\sigma}{d\Omega} = \frac{1}{4k^4}\left(\frac{1}{\sin^4\chi/2} + \frac{1}{\cos^4\chi/2}\right) \tag{149}$$

The cross-section for scattering at small and large angles is highly divergent. The cross-section can be defined only when the center-of-mass motion is at rest. The particles are identical and have equal kinetic energies $p_1^2 = p_2^2$ due to the statistics, and there is no reference frame where only one of the particles is at rest. This also means that the problem does not exhibit spherical rotation symmetry, instead it exhibits cylindrical rotation symmetry.

II. CONCLUSION

We show that in the particular case of systems with two particles, that the constraints of particle identity entail reduction in the number of internal degrees-of-freedom from six to five. The effect of redundancy in the description of orbital motion in the two-particle gauge system is found to be in correspondence with the multiplicative phase-factor $(-1)^S$, where $S = \{0, 1\}$ is the total spin.

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